

Effect of phase fluctuations on INS and NMR experiments in the pseudo-gap regime of the underdoped cuprates

Harry Westfahl Jr.¹ and Dirk K. Morr^{1,2}

¹ *University of Illinois at Urbana-Champaign, Loomis Laboratory of Physics, 1110 W. Green St., Urbana, IL 61801*

² *Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545*

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We present a theory for inelastic neutron scattering (INS) and nuclear magnetic resonance (NMR) experiments in the pseudo-gap regime of the underdoped high- T_c cuprates. We show that superconducting phase fluctuations greatly affect the temperature and frequency dependence of the spin-susceptibility, χ'' , probed by both experimental techniques. This result explains the appearance of a *resonance peak*, observed in INS experiments, below a temperature $T_0 > T_c$. In the same temperature regime, we find that the ^{63}Cu spin-lattice relaxation rate, $1/T_1$, measured in NMR experiments, is suppressed. Our results are in qualitative agreement with the available experimental data.

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Over the last few years intensive research has focused on the origin of the pseudo-gap region in the underdoped high- T_c cuprates [1–7]. This part of the phase diagram, below a characteristic temperature $T_* > T_c$, is characterized by a suppression of the low-frequency quasi-particle spectral density, as observed by angle-resolved photo-emission (ARPES) [8] and scanning tunneling spectroscopy (STS) experiments [9]. For the same compounds, inelastic neutron scattering (INS) experiments have revealed a sharp magnetic mode, the *resonance peak*, below T_* , in contrast to the optimally doped cuprates, where it only appears below T_c [10]. Moreover, nuclear magnetic resonance (NMR) experiments find a strong decrease of the ^{63}Cu spin-lattice relaxation rate, $1/T_1$, below T_* [11,12].

These experimental observations put tight restrictions on the proposed theoretical scenarios for the pseudogap ascribing it to spin-charge separation [7], SO(5) symmetry [6], condensation of preformed pairs [5] and spin-fluctuations [4]. Emery and Kivelson (EK) [1] proposed that, due to the small superfluid density of the underdoped cuprates, thermal fluctuations in the phase of the superconducting (SC) order parameter destroy the long-range phase coherence in the pseudo-gap regime, while preserving a finite local amplitude of the order parameter, $|\Delta(r)|$. In this communication, we argue that the presence of phase fluctuations provides an explanation for the results of INS and NMR experiments discussed above. We show that these fluctuations greatly affect the temperature and frequency dependence of the spin-susceptibility, χ'' , probed by both experimental techniques. Support for the existence of phase fluctuations comes from recent high frequency transport experiments by Corson *et al.* [13]. They demonstrated that the SC transition in underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8-\delta}$ (Bi-2212) is of the Kosterlitz-Thouless (KT) type, where at $T_c = 74\text{K}$ the unbinding of thermally excited vortex-anti-vortex pairs destroys the long-range phase coherence. However, they also concluded that $|\Delta(r)|$ vanishes at a temperature $T_0 \sim 100\text{K}$, while the onset temperature, T_* , for

the pseudo-gap regime is much higher. For this reason we will focus our analysis on the region $T_c < T < T_0$.

The starting point for our calculations is the mean-field BCS Hamiltonian in which the phase, $\theta(r)$, of the superconducting order parameter, $\Delta(r) = |\Delta(r)|e^{i\theta(r)}$, varies on the scale of the phase coherence length, ξ_θ . Such a nonuniform phase $\theta(\mathbf{r})$ is treated via a gauge transformation [2,3]

$$\Psi^\dagger = e^{i\theta(r)/2} c^\dagger \quad (1)$$

where c^\dagger is the creation operator of the original electrons. This transformation induces a coupling of the Ψ -fermions to a local superfluid flow $\mathbf{v}_s(\mathbf{r}) = \nabla\theta(\mathbf{r})/2\mathbf{m}$, (we set $\hbar = 1$) whose thermodynamic properties are determined by the 2D-XY Hamiltonian

$$\frac{\mathcal{H}_{XY}}{k_B T} = \frac{K_0(T)}{2} \int d^2\mathbf{r} |\nabla\theta(\mathbf{r})|^2, \quad (2)$$

where $K_0(T) = n_s(T)/(4mk_B T)$ is the “bare” phase stiffness and $n_s(T)$ is the 2D superfluid density per CuO_2 layer which for a d-wave superconductor is given by $n_s(T) = n_s(0)(1 - T/T_0)$, where T_0 is the BCS mean field temperature [7]. In order to compute χ'' in the presence of phase fluctuations we first compute it for a given configuration of $\mathbf{v}_s(\mathbf{r})$ and subsequently perform a thermodynamic average over the ensemble specified by Eq.(2). Our approach is similar to the one adopted by Franz and Millis (FM) [2] who computed the single particle Green’s function, $G(k, \omega)$, in the pseudo-gap regime. They showed that the quantity which determines the ensemble average is the correlator $W = m^2 v_F^2 \langle \mathbf{v}_s^2 \rangle / 2$, whose temperature dependence they extracted from fits to ARPES and STS experiments. In the following we show that $W(T)$ can also be obtained from the experiments by Corson *et al.* [13]

Assuming that the superfluid velocity is purely due to transverse phase fluctuations, we have

$$W(T) = \pi^2 v_F^2 \int \frac{d^2\mathbf{q}}{4\pi^2} \frac{G(\mathbf{q})}{q^2}, \quad (3)$$

where $G(\mathbf{q}) = \langle \mathbf{n}_\mathbf{q} \mathbf{n}_{-\mathbf{q}} \rangle$ is the vortex density correlator. In the limit of large vortex density, this correlator is given by [14] $G(\mathbf{q})^{-1} \sim 4\pi^2 K_0(\xi_\theta^2 + q^{-2})$. Evaluation of the integral in Eq.(3) with wave-vector cutoff $\Lambda = 2\pi\xi_{GL}^{-1}$ yields

$$W(T) \simeq \frac{\pi^3 \Delta_0^2}{8K_0(T)} \left(\frac{\xi_{GL}}{2\pi\xi_\theta} \right)^2 \ln \left[1 + \left(\frac{2\pi\xi_\theta}{\xi_{GL}} \right)^2 \right]. \quad (4)$$

Here, the phase coherence length is given by $\xi_\theta^{-2}(T) = 4\pi^2 K_0(T) n_F(T)$, where $n_F(T)$ is the density of free vortices, and we used the BCS result $\xi_{GL} = v_F/(\pi\Delta_0)$. Corson *et al.* found in their analysis that $n_F(T) = (2A/\pi\xi_{GL}^2) \exp(-8CK_0(T))$ with A and C being constants of order $O(1)$. Assuming that the functional form of $n_F(T)$ (and thus that of $W(T)$) remains the same for all underdoped Bi-2212 compounds, with A and C being the only doping dependent parameters, we present $W(T)$ from Eq.(4) in the inset of Fig. 2, together with FM's fits [2] to STS experiments in Bi-2212 ($T_c = 83K$) [9]. With $A = 0.1$ and $C = 0.6$, we find good quantitative agreement of our theoretical results with those of FM up to $T_0 \approx 150$ K. At this temperature, the above approximation, as well as the analysis by FM, presumably break down since $\sqrt{W(T)}$ becomes of the order of the maximum superconducting gap.

We now turn to the appearance of the resonance peak in the pseudogap region. Morr and Pines (MP) [15] recently argued that the resonance peak in the superconducting state arises from a spin-wave mode whose dispersion is given by

$$\omega_q^2 = \Delta_{sw}^2 + c_{sw}^2 |\mathbf{q} - \mathbf{Q}|^2, \quad (5)$$

where Δ_{sw} is the spin-wave gap, c_{sw} is the spin-wave velocity and \mathbf{Q} is the position of the magnetic peak in momentum space. Starting from a spin-fermion model [16], MP showed that this mode is strongly damped in the normal state, but becomes only weakly damped in the superconducting state, if Δ_{sw} is less than the gap, ω_c , for particle-hole excitations with total momentum \mathbf{Q} . These excitations connect points on the Fermi surface (FS) in the vicinity of $(0, \pi)$ and $(\pi, 0)$ ("hot spots"), and thus for a d-wave gap $\Delta_{\mathbf{k}} = \Delta_0 (\cos(k_x) - \cos(k_y))/2$, $\omega_c \approx 2\Delta_0$.

MP computed χ using the Dyson-equation

$$\chi^{-1} = \chi_0^{-1} - \Pi, \quad (6)$$

where χ_0 is the "bare" susceptibility and Π is the bosonic self-energy given by the irreducible particle-hole bubble. For χ_0 , MP made the experimentally motivated ansatz

$$\chi_0^{-1} = \frac{\omega_q^2 - \omega^2}{\alpha c_{sw}^2}, \quad (7)$$

where ω_q is given in Eq.(5). In the superconducting state, one obtains for Π to lowest order in the spin-fermion coupling g

$$\begin{aligned} \Pi(\mathbf{q}, i\omega_n) = & -g^2 T \sum_{\mathbf{k}, m} \left\{ G(\mathbf{k}, i\Omega_m) G(\mathbf{k} + \mathbf{q}, i\Omega_m + i\omega_n) \right. \\ & \left. + F(\mathbf{k}, i\Omega_m) F(\mathbf{k} + \mathbf{q}, i\Omega_m + i\omega_n) \right\}, \quad (8) \end{aligned}$$

with G and F being the normal and anomalous Green's functions. Since, within the spin-fermion model, χ_0 is obtained by integrating out the high-energy fermionic degrees of freedom, it is largely unaffected by the onset of superconductivity or the pseudo-gap. Moreover, MP argued that due to fermionic self-energy corrections, $\text{Re } \Pi$ in the SC state only leads to an irrelevant renormalization of Δ_{sw} and c_{sw} . Since the same argument also holds within our scenario for the pseudo-gap region, we neglect $\text{Re } \Pi$ in the following.

On the other hand, $\text{Im } \Pi$ which determines the damping of the spin excitations, changes dramatically in the SC state due to the opening of a gap in the fermionic dispersion. Consequently, we expect phase fluctuations to strongly affect $\text{Im } \Pi$. Moreover, in each polarization bubble present in the RPA expansion of Eq.(6), the electron-hole pairs probe different parts of the sample and thus independent configurations of thermally excited supercurrents. It then follows that the susceptibility, χ_{pf} , in the presence of phase fluctuations is obtained from Eq.(6) by using $\text{Im } \Pi_{pf}$ averaged over the thermodynamic ensemble determined by Eq.(2).

Before we discuss the effect of phase fluctuations on $\text{Im } \Pi$, we shortly review its form in the normal and SC state. Extending Eq.(8) to the normal state, we obtain $\text{Im } \Pi(\mathbf{Q}) = 4g^2\omega/(\pi v_F^2)$ [17], where v_F is the Fermi velocity at the hot spots. In contrast, in the SC state, in the limit of $T \ll \omega_c$, we find to order $O(T/\omega_c)$

$$\begin{aligned} \text{Im } \Pi(\mathbf{Q}, \omega) = & \frac{4g^2\omega_c}{\pi v_F^2} E(\sqrt{1 - \bar{\omega}^2}) \theta(\bar{\omega} - 1) \\ \sim & \frac{g^2\omega_c}{v_F^2} (\bar{\omega} + 1) \theta(\bar{\omega} - 1), \quad (9) \end{aligned}$$

where $\theta(x)$ is the Heavyside step function, $E(x)$ is the complete Elliptic integral of the first kind and $\bar{\omega} = \omega/\omega_c$. Thus, $\text{Im } \Pi$ vanishes for frequencies below ω_c . In Fig. 1 we present the frequency dependence of $\text{Im } \Pi$ in the normal and SC state.

We now consider the effect of phase fluctuations on $\text{Im } \Pi$. Note that Π , Eq.(8), and thus χ , Eq.(6), are invariant under the gauge transformation, Eq.(1), in contrast to $G(k, \omega)$, considered by FM. Thus G, F can be straightforwardly calculated using the Ψ -fermions. In the limit $k_F \xi_\theta \gg 1$, where k_F is the Fermi momentum at the hot-sp

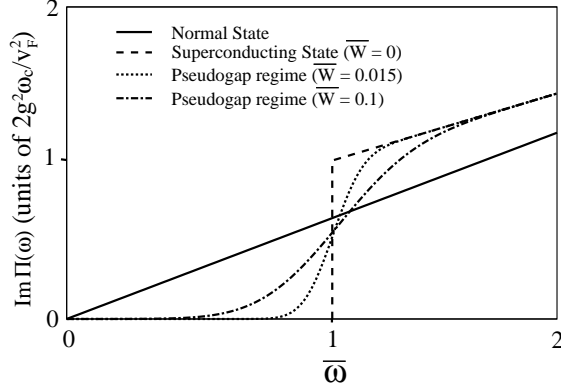


FIG. 1. $\text{Im } \Pi$ in the normal (black line) and SC state (dashed line), and $\text{Im } \Pi_{pf}(\omega)$ in the pseudo-gap region for (a) $\bar{W} = 0.015$ (dotted line), and (b) $\bar{W} = 0.1$ (dashed-dotted line).

is the Fermi velocity. In the limit $T \ll D_{\mathbf{k}} \ll \Delta_0$, $\text{Im } \Pi$ for a given superfluid velocity is obtained from Eq.(9) via the frequency shift

$$\omega \rightarrow \omega + (D_x + D_y) . \quad (11)$$

Similar to the case of the fermionic spectral function [2], the thermodynamic average of $\text{Im } \Pi$ over the ensemble specified by Eq.(2) is obtained by convoluting $\text{Im } \Pi$ with a Gaussian distribution of Doppler shifts of the form

$$P(D_\alpha) = \frac{1}{\sqrt{2\pi W}} \exp\left(-\frac{D_\alpha^2}{2W}\right) , \quad (12)$$

where $\alpha = x, y$. In the limit $\sqrt{W} \ll T \ll \omega_c$, we can perform this convolution analytically and obtain

$$\begin{aligned} \text{Im } \Pi_{pf}(\omega) = \frac{g^2 \omega_c}{2v_F^2} \left\{ (1 + \bar{\omega}) \left[1 + \Phi\left(\frac{\bar{\omega} - 1}{\sqrt{\bar{W}(T)}}\right) \right] \right. \\ \left. + \sqrt{\bar{W}(T)/\pi} \exp\left(-\frac{(\bar{\omega} - 1)^2}{\bar{W}(T)}\right) \right\} , \quad (13) \end{aligned}$$

where $\Phi(x)$ is the error function. It follows from Fig. 1, in which we present the spin-damping for two different values of $\bar{W} = W/\Delta_0^2$, that the effect of phase fluctuations on $\text{Im } \Pi$ is two-fold. First, they lead to a non-zero value of $\text{Im } \Pi_{pf}(\omega)$ for $\omega < \omega_c$, in contrast to the form of $\text{Im } \Pi$ in the superconducting state where the spin-damping at $T = 0$ vanishes below ω_c . Second, the spin-damping below ω_c increases with increasing W while at the same time, the sharp step in $\text{Im } \Pi$ is smoothed out. Note that in the pseudo-gap region, $T \ll \omega_c$, and consequently the temperature dependence of $\text{Im } \Pi_{pf}(\omega)$ is determined by that of $W(T)$.

Finally, inserting $\text{Im } \Pi_{pf}(\omega)$ into Eq.(6), we obtain $\chi''_{pf}(\mathbf{Q}, \omega)$ in the pseudo-gap region. In Fig. 2 we present

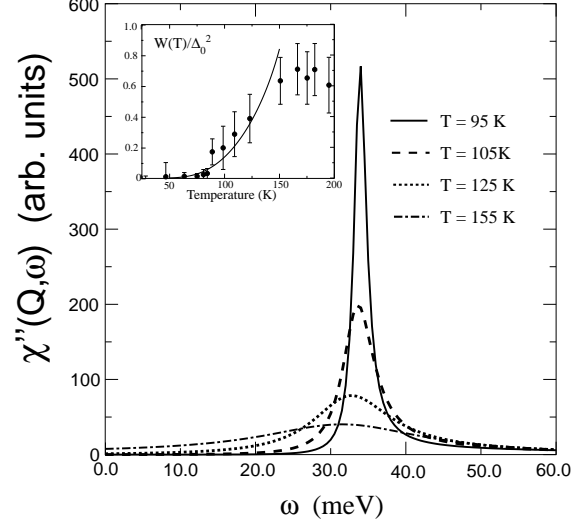


FIG. 2. The resonance peak in the pseudo-gap region for $\frac{g^2 \alpha \xi^2}{2v_F^2} = 1/(70 \text{ meV})$, $\Delta_{sw} = 35 \text{ meV}$, $\omega_c = 65 \text{ meV}$ and $W(T)$ from the inset. Inset: $W(T)$ from Ref. [2] (points) and from Eq.(4) with $A=0.1$ and $C=0.6$ (solid line).

our theoretical results for the frequency and temperature dependence of the resonance peak in Bi-2212 ($T_c = 83 \text{ K}$), using the $W(T)$ shown on the inset. We find that, as the temperature is increased above T_c , the resonance peak becomes broader, while its intensity diminishes. Since $W(T)$ is a monotonically increasing function of temperature, it follows from Fig. 1 that the spin damping for $\omega \approx \Delta_{sw} < \omega_c$ also increases with temperature, giving rise to the behavior of the peak intensity/width shown in Fig. 2. Unfortunately, no experimental data for the temperature dependence of the resonance peaks in the pseudo-gap region of underdoped Bi-2212 are currently available. However, our results are in qualitative agreement with the experimental data on underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ [10].

We now turn to the second experimental probe of χ'' , the ^{63}Cu spin-lattice relaxation rate, $1/T_1$. For an applied field parallel to the c -axis, $1/T_1$ is given by

$$\frac{1}{T_1 T} = \frac{k_B}{2} (\gamma_n \gamma_e)^2 \frac{1}{N} \sum_{\mathbf{q}} F_c(\mathbf{q}) \lim_{\omega \rightarrow 0} \frac{\chi''(\mathbf{q}, \omega)}{\omega} , \quad (14)$$

where

$$F_c(\mathbf{q}) = [A_{ab} + 2B (\cos(q_x) + \cos(q_y))]^2 , \quad (15)$$

and A_{ab} and B are the on-site and transferred hyperfine coupling constants, respectively. The spin-lattice relaxation rate in the mixed state, i.e., in the presence of a superflow, was recently considered by Morr and Worris (MW) [18]. Using the low-frequency limit of Eqs.(6) and (8), they found that the temperature dependence of $1/T_1$ is determined by the set $\{D_n/T\}$, where D_n is the

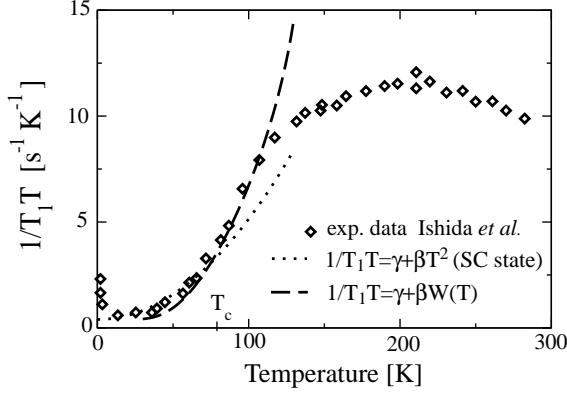


FIG. 3. $1/T_1T$ in the pseudo-gap region of underdoped Bi-2212 ($T_c = 79K$). Solid line: theoretical fits with $A=0.05$ and $C=0.3$. Filled squares: experimental data taken from Ref. [12]. We assumed a constant background factor $\gamma = 0.4K^{-1}s^{-1}$

Doppler-shift at the n th node (see Eq.(10)). In the limit, $|D_n/T| \gg 1$, they obtained

$$\frac{1}{T_1T} = \frac{C}{N} \sum_{i,j} \mathcal{F}(\mathbf{q}_{i,j}) |D_i| |D_j|, \quad (16)$$

where $C = (k_B/\pi)(\alpha g \gamma_n \gamma_e)^2 / (4v_F v_\Delta)^2$, $v_\Delta = |\partial \Delta_{\mathbf{k}} / \partial \mathbf{k}|$ at the nodes, and

$$\mathcal{F}(\mathbf{q}_{i,j}) = \frac{F_c(\mathbf{q}_{i,j})}{(\xi^{-2} + |\mathbf{q}_{i,j} - \mathbf{Q}|^2)^2}. \quad (17)$$

Here, $\mathbf{q}_{i,j}$ is the wave-vector connecting the nodes i and j , and ξ is the magnetic correlation length. In the limit $T \ll \sqrt{W(T)}$, the convolution of Eq.(16) with the Gaussian distribution of Eq.(12) can be performed analytically, and we obtain

$$\left(\frac{1}{T_1T} \right)_{pf} = \beta W(T) \quad (18)$$

where $\beta = 4C(\mathcal{F}(0) + \mathcal{F}(\mathbf{q}_{1,3}) + \frac{8}{\pi}\mathcal{F}(\mathbf{q}_{1,2}))$. The constant β can be experimentally obtained [19] by fitting $(T_1T)^{-1}$ at $T < T_c$ with the d-wave BCS expression $(T_1T)^{-1} = \beta \frac{\pi^2}{3} T^2$. Note that the relaxation rate in Eq.(18) directly reflects the strength of the classical phase fluctuations. In Fig. 3 we present our theoretical results for $(T_1T)^{-1}_{pf}$, Eq.(18), together with the experimental data by Ishida *et al.* [12] on underdoped Bi-2212 ($T_c = 79K$). Using $W(T)$, Eq.(4), with $A=0.05$ and $C=0.3$, we find good agreement of our theoretical results with the experimental data between T_c and $T_0 \approx 130$ K. Note that the external magnetic field applied in NMR experiments increases the density of free vortices by $\bar{n}_F(B) \sim B/\phi_0$ [14]. As a result, the phase coherence length (and in turn W) acquires a magnetic field dependence, $\xi_\theta^{-2} = 4\pi^2 K_0(T) (n_F(T) + \bar{n}_F(B))$. For $T \geq T_c$,

and the parameter set used above, we find that a magnetic field of $B = 10T$ increases the vortex density by $\bar{n}_F(B)/n_F(T_c) \sim 0.1$; its contribution to W can thus be neglected. Thus the relaxation rate above T_c should be independent of magnetic field for typical values of B , which is consistent with recent experiments by Gorny *et al.* [21].

In the above scenario, we neglected the effect of longitudinal phase fluctuations which arise from spin-wave like excitations. This is justified since their excitation spectrum is very likely gapped by the Anderson-Higgs mechanism [2], and they are, consequently, irrelevant for the low-frequency thermodynamic properties of the underdoped cuprates. It was recently proposed in Ref. [22] that longitudinal phase fluctuations are responsible for the linear temperature dependence of the superfluid density at $T \ll T_c$. FM pointed out that longitudinal phase fluctuations at $T \ll T_c$ lead to a $W_{long} \sim T$. In this case it follows from Eq.(18) that, for ^{63}Cu and ^{17}O , $1/T_1T \sim T$ at $T \ll T_c$, in contrast to the experimentally observed $1/T_1T \sim T^2$ [23]. This result suggests that longitudinal phase fluctuations are absent in the superconducting state.

We assumed above, following the argument applied to STS and ARPES experiments [2], that transverse phase fluctuations are static on the time-scale of INS and NMR experiments which allowed us to neglect the quantum dynamical nature of the vortices. While this assumption likely holds for “fast” probes like INS, ARPES and STS where the quasi-particles are coupled to phase fluctuations for short times, it might be less justified for the much “slower” NMR experiments. In this light, the agreement of our theoretical NMR results with the experimental data, Fig. 3 is remarkable. However, the effects of the vortex quantum dynamics on various experimental probes is still an open question which requires further study.

In summary we propose a scenario for INS and NMR experiments in the pseudogap region of the underdoped cuprates. We argue that phase fluctuations of the superconducting order parameter drastically affect the frequency dependence of the spin susceptibility and can thus qualitatively account for the temperature dependence of the resonance peak. Moreover, we show that the spin-lattice relaxation rate, $1/T_1T$, is a direct probe for the strength of the phase fluctuations, as reflected in $W(T)$. Finally, we showed that $W(T)$ obtained from high frequency transport measurements is in good qualitative agreement with that extracted from STS experiments.

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